

Ethyl heptanoate
106-30-9 | DTXSID1040112

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -63.0 °C

Global applicability domain: Inside

Local applicability domain index: 9.92e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl heptanoate</div> <div>Measured: -66.1</div> <div>Predicted: -63.0</div>	<div>Image not found</div> <div>Heptyl acetate</div> <div>Measured: -50.2</div> <div>Predicted: -56.4</div>	<div>Image not found</div> <div>Hexyl propanoate</div> <div>Measured: -57.5</div> <div>Predicted: -71.4</div>
<div>Image not found</div> <div>Propyl hexanoate</div> <div>Measured: -68.7</div> <div>Predicted: -71.7</div>	<div>Image not found</div> <div>Pentyl butyrate</div> <div>Measured: -73.2</div> <div>Predicted: -72.0</div>	